A METHOD FOR PROTEIN STRUCTURE ALIGNMENT

ABSTRACT OF THE DISCLOSURE

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This invention provides a method for protein structure alignment. More particularly, the present invention provides a method for identification, classification and prediction of protein structures. The present invention involves two key ingredients. First, an energy or cost function formulation of the problem simultaneously in terms of binary (Potts) assignment variables and real-valued atomic coordinates. Second, a minimization of the energy or cost function by an iterative method, where in each iteration (1) a mean field method is employed for the assignment variables and (2) exact rotation and/or translation of atomic coordinates is performed, weighted with the corresponding assignment variables.

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